The hidden talents of logistic regression

From noisy labels to point processes

Aditya Krishna Menon





November 7th, 2017

Three problems...





Three problems...one solution?





Three problems...one solution?



Fairness

DRE applications



Covariate shift



Outlier detection



Robot transition estimation

DRE applications



Covariate shift



Outlier detection



Robot transition estimation

In some cases, a different view may be more natural

Class-probability estimation (CPE) From labelled instances



Class-probability estimation (CPE)

From labelled instances, estimate probability of instance being +'ve

• e.g. using logistic regression



This talk



This talk

A formal link between DRE and CPE



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CPE approach to three distinct learning problems



Class-probability estimation

Distributions for learning with binary labels

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$$(P(x), Q(x)) = (\mathbb{P}(\mathsf{X} = x \mid \mathsf{Y} = +1), \mathbb{P}(\mathsf{X} = x \mid \mathsf{Y} = -1))$$
$$(M(x), \eta(x)) = (\mathbb{P}(\mathsf{X} = x), \mathbb{P}(\mathsf{Y} = +1 \mid \mathsf{X} = x))$$



Marginal and class-probability function



Scorers, losses, risks

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• e.g. linear scorer $s: x \mapsto \langle w, x \rangle$



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The risk of scorer s wrt loss ℓ and distribution D is

 $\mathop{\mathbb{E}}_{(\mathsf{X},\mathsf{Y})\sim D}[\ell(\mathsf{Y},s(\mathsf{X}))]$



average loss on a random sample

For suitable $\mathbb{S} \subset \mathbb{R}^{\mathcal{X}},$ minimise empirical risk

$$\operatorname{argmin}_{s\in\mathbb{S}}\frac{1}{N}\sum_{n=1}^{N}\ell(y_n,s(x_n))$$

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Estimate $\hat{\boldsymbol{\eta}} \doteq \Psi^{-1} \circ s$

• e.g. for logistic loss, $\hat{\eta}(x) = 1/(1 + \exp(-s(x)))$

Examples of proper composite losses





Logistic loss

 $\Psi^{-1} \colon v \mapsto 1/(1 + \exp(-v))$



$$\Psi^{-1}: v \mapsto 1/(1 + \exp(-2v))$$



 $\Psi^{-1}: v \mapsto \min(\max(0,(v+1)/2),1)$

Class-probabilities and density ratios

CPE versus DRE

Given samples $S \sim D^N$, with $D = (P, Q) = (M, \eta)$:

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class-probability function



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Density ratio estimation (DRE) Estimate r = p/q

class-conditional density ratio



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$$= \frac{\eta(x)}{1 - \eta(x)}$$

Bayes' rule shows DRE and CPE are linked (Bickel et al, 2009):

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But what about approximate solutions?

CPE and DRE: approximate solutions?

Natural class-probability estimate: $\hat{\boldsymbol{\eta}} \doteq \Psi^{-1} \circ s$

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Intuitive, but what can we guarantee about this?

For proper composite ℓ , the regret of a scorer is

$$\operatorname{reg}(s) \doteq \mathbb{E}\left[\ell(\mathsf{Y}, s(\mathsf{X}))\right] - \min_{\overline{s} \in \mathbb{R}^{\mathcal{X}}} \mathbb{E}\left[\ell(\mathsf{Y}, \overline{s}(\mathsf{X}))\right]$$

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Is there a similar sense in which \hat{r} is reasonable?

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CPE implicitly estimates density ratios

complementary to (Sugiyama et al., 2012)

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Underlying Bregman identity has multi-dimensional generalisation

Nock et al. A scaled Bregman theorem with applications. NIPS 2016.

Summary thus far



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Learning from noisy binary labels

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Learning from noisy binary labels

















Label noise: formally

We care about "clean" D

$\underset{s}{\underset{(\mathbf{X},\mathbf{Y})}{\text{Ideal}}} \mathbb{E}\left[\ell(\mathbf{Y},s(\mathbf{X}))\right]$

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We care about "clean" D, but observe samples from $\overline{D} \neq D$

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 $\begin{array}{c} \textbf{Ideal} \\ \min_{s} \mathop{\mathbb{E}}_{(\mathsf{X},\mathsf{Y})} \left[\ell(\mathsf{Y}, s(\mathsf{X})) \right] \end{array}$



How to minimise the ideal risk?

Denote by $\eta(x)$ the "clean" $\mathbb{P}(Y = +1 | X = x)$

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We may write

$$\begin{bmatrix} \bar{\boldsymbol{\eta}}(x) \\ 1 - \bar{\boldsymbol{\eta}}(x) \end{bmatrix} = \underbrace{\begin{bmatrix} 1 - \rho & \rho \\ \rho & 1 - \rho \end{bmatrix}}_{T} \begin{bmatrix} \boldsymbol{\eta}(x) \\ 1 - \boldsymbol{\eta}(x) \end{bmatrix}$$

 $\mathop{\mathbb{E}}_{(\mathsf{X},\mathsf{Y})}[\ell(\mathsf{Y},s(\mathsf{X}))]$

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for the noise-corrected loss (Natarajan et al., 2013)

$$\overline{\ell}(y,v) = \frac{1}{1-2\cdot\rho} \left((1-\rho) \cdot \ell(y,v) - \rho \cdot \ell(-y,v) \right)$$

$$\begin{split} & \underset{(\mathbf{X},\mathbf{Y})}{\mathbb{E}} \left[\ell(\mathbf{Y}, s(\mathbf{X})) \right] = \underset{\mathbf{X} \sim M}{\mathbb{E}} \begin{bmatrix} \eta(\mathbf{X}) \\ 1 - \eta(\mathbf{X}) \end{bmatrix}^{\mathrm{T}} \left[\ell(+1, s(\mathbf{X})) \quad \ell(-1, s(\mathbf{X})) \right] \\ &= \underset{\mathbf{X} \sim M}{\mathbb{E}} \begin{bmatrix} \bar{\eta}(\mathbf{X}) \\ 1 - \bar{\eta}(\mathbf{X}) \end{bmatrix}^{\mathrm{T}} (T^{-1})^{\mathrm{T}} \left[\ell(+1, s(\mathbf{X})) \quad \ell(-1, s(\mathbf{X})) \right] \\ &= \underset{\mathbf{X} \sim M}{\mathbb{E}} \begin{bmatrix} \bar{\eta}(\mathbf{X}) \\ 1 - \bar{\eta}(\mathbf{X}) \end{bmatrix}^{\mathrm{T}} \left[\bar{\ell}(+1, s(\mathbf{X})) \quad \bar{\ell}(-1, s(\mathbf{X})) \right] \\ &= \underset{(\mathbf{X}, \bar{\mathbf{Y}})}{\mathbb{E}} \left[\bar{\ell}(\bar{\mathbf{Y}}, s(\mathbf{X})) \right], \end{split}$$

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But ρ is unknown...

Noise rate estimation

One can avoid knowing ho for suitable ℓ

• eigenfunctions for the loss transform, e.g. "un-hinged" loss

van Rooyen et al. Learning with symmetric label noise: the importance of being unhinged. NIPS 2015. Menon et al. Learning from corrupted binary labels via class-probability estimation. ICML 2015.

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Alternately, assume $\min_x \eta(x) = 0$, $\max_x \eta(x) = 1$

- "guaranteed" positive and negative instances
- c.f. (Scott et al., 2013), (du Plessis et al., 2014)

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Since $\overline{\eta}(x) = (1 - 2 \cdot \rho) \cdot \eta(x) + \rho$,

 $\min_{x} \overline{\eta}(x) = \rho \qquad \max_{x} \overline{\eta}(x) = 1 - \rho$

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Range of $\bar{\eta}$ lets us estimate ρ !

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Beyond symmetric binary noise

For asymmetric multi-class noise, we similarly have

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where e.g. $\overline{\eta}(x) = (\mathbb{P}(\mathsf{Y} = 1 \mid \mathsf{X} = x), \dots, \mathbb{P}(\mathsf{Y} = K \mid \mathsf{X} = x))$

analogous noise-corrected loss and noise estimation

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analogous noise-corrected loss and noise estimation

Broader range of weakly supervised problems captured

• confer (van Rooyen & Williamson, 2017)

Illustration: deep network

Corrected losses with and without noise estimation



Patrini et al. Making deep neural networks robust to label noise: a loss correction approach. CVPR 2017.

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Suppose (x, y) has label flipped with probability $\rho(x) \in [0, 1/2)$

The "noisy" class-probability function is

$$\overline{\boldsymbol{\eta}}(x) = (1 - \boldsymbol{\rho}(x)) \cdot \boldsymbol{\eta}(x) + \boldsymbol{\rho}(x) \cdot (1 - \boldsymbol{\eta}(x))$$

Denote by $\eta(x)$ the "clean" $\mathbb{P}(\mathsf{Y} = +1 \mid \mathsf{X} = x)$

Suppose (x,y) has label flipped with probability $\rho(x) \in [0,1/2)$

The "noisy" class-probability function is

$$\overline{\boldsymbol{\eta}}(x) = (1 - \boldsymbol{\rho}(x)) \cdot \boldsymbol{\eta}(x) + \boldsymbol{\rho}(x) \cdot (1 - \boldsymbol{\eta}(x))$$

Estimating $\rho(x)$ is non-trivial

• To make progress, we impose some structure on ρ and η

Assumptions on noise and distribution

Noise increases as $\eta(x)$ approaches 1/2

• higher inherent uncertainty \rightarrow higher noise

Assumptions on noise and distribution

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Class-probability is expressible as

$$\boldsymbol{\eta}(x) = \boldsymbol{u}(\langle w^*, x \rangle)$$

for some non-decreasing, Lipschitz $u(\cdot)$

- u unknown \rightarrow single index model (SIM)
- such models learnable via Isotron (Kalai & Sastry, 2009)

Structure of noisy class-probability

Under these assumptions, one may show

 $\bar{\boldsymbol{\eta}}(x) = \bar{\boldsymbol{u}}(\langle w^*, x \rangle)$

for monotone \overline{u}

- still in the SIM family!
- noise is baked into \overline{u}

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Under these assumptions, one may show

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- noise is baked into \overline{u}

One can estimate $\bar{\eta}$ via Isotron

• do not need to know flip function ρ or link function u

Illustration: instance-dependent noise

Label flip function $f(z) = (1 + e^{|z|/\alpha})^{-1}$

α	Ridge ACC	Isotron ACC
$\frac{\frac{1}{8}}{\frac{1}{4}}$ $\frac{1}{2}$ 1 2 4 8	$\begin{array}{c} 0.9940 \pm 0.0003\\ 0.9947 \pm 0.0004\\ 0.9944 \pm 0.0004\\ 0.9853 \pm 0.0012\\ 0.8988 \pm 0.0053\\ 0.7410 \pm 0.0072\\ 0.6185 \pm 0.0078\\ \end{array}$	$\begin{array}{c} 0.9974 \pm 0.0002 \\ 0.9974 \pm 0.0003 \\ 0.9937 \pm 0.0006 \\ 0.9700 \pm 0.0021 \\ 0.9239 \pm 0.0050 \\ 0.7863 \pm 0.0138 \\ 0.6467 \pm 0.0405 \end{array}$

α	Ridge ACC	Isotron ACC
$\frac{1}{8}$	0.9958 ± 0.0001	0.9984 ± 0.0001
$\frac{\overline{4}}{1}$	$\begin{array}{c} 0.9958 \pm 0.0001 \\ 0.9953 \pm 0.0002 \end{array}$	$\begin{array}{c} 0.9979 \pm 0.0001 \\ 0.9966 \pm 0.0003 \end{array}$
1	0.9871 ± 0.0005	0.9864 ± 0.0007
2	0.9446 ± 0.0012	0.9565 ± 0.0013
4	0.8262 ± 0.0022	0.8768 ± 0.0041
8	0.6872 ± 0.0024	0.8088 ± 0.0291

usps 0v9

mnist 6v7

Summary thus far



Fitting point processes

Point processes

Model the rate at which events occur in time

• re-tweets in a social network, earthquakes, ...



Point processes: formally

Suppose $(N(t))_{t\geq 0}$ counts the # of events in (0, t]

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In the non-homogeneous Poisson process (NHPP), one posits that the # of events in (s, t] follows

$$N(t) - N(s) \sim Poiss\left(\int_{s}^{t} \lambda(u) du\right)$$

for intensity function $\lambda \colon \mathbb{R}_+ \to \mathbb{R}_+$

instantaneous rate at which events occur

Suppose we observe event times $\{t_1, \ldots, t_N\}$, with $T \doteq \max_n t_n$

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The negative log-likelihood for intensity $\lambda(\cdot;\theta)$ is

$$\mathcal{L}(\boldsymbol{\theta}) \doteq \sum_{n=1}^{N} -\log \lambda(t_n; \boldsymbol{\theta}) + \int_0^T \lambda(u; \boldsymbol{\theta}) \,\mathrm{d}u$$

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$$= \sum_{\mathsf{T} \sim \hat{\boldsymbol{P}}} \left[-\log \lambda(\mathsf{T}; \boldsymbol{\theta}) \right] + \frac{T}{N} \cdot \sum_{\mathsf{T}' \sim \boldsymbol{Q}} \left[\lambda(\mathsf{T}'; \boldsymbol{\theta}) \right]$$

where Q is uniform over [0, T]

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Classification with a uniform background!

On an interval [0,T], event times $\{t_1,\ldots,t_N\}$ are iid with density

$$p(t) = \frac{\lambda(t)}{\int_0^T \lambda(u) \, \mathrm{d}u}$$

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$$\underset{\lambda \in \mathbb{R}^{\mathcal{X}}_{+}}{\operatorname{argmin}} \mathbb{E}_{P}\left[-\log \lambda(\mathsf{T})\right] + \frac{T}{N} \cdot \mathbb{E}_{Q}\left[\lambda(\mathsf{T}')\right] = N \cdot p$$

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Weighted density ratio estimation!

Generalised likelihood?

For scorer $s \colon \mathbb{R}_+ \to \mathbb{R}$, consider

$$\min_{s \in \mathcal{S}} \mathbb{E} \left[\ell(+1, s(\mathsf{T})) \right] + \frac{T}{N} \cdot \mathbb{E} \left[\ell(-1, s(\mathsf{T}')) \right]$$
$$= \min_{s \in \mathcal{S}} \sum_{n=1}^{N} \ell(+1, s(t_n)) + \int_{0}^{T} \ell(-1, s(t)) \, \mathrm{d}t$$

for strictly proper composite ℓ

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for strictly proper composite ℓ

We retain the optimal solution by picking

$$\lambda(t) = rac{\Psi^{-1}(s(t))}{1 - \Psi^{-1}(s(t))}$$

• optimal
$$s = \Psi(\eta), \frac{\eta}{1-\eta} \propto p$$

Application: Hawkes processes

The self-exciting Hawkes process assumes, for link $F(\cdot)$,

$$\lambda\left(t; \{t_n\}_{n=1}^N\right) = F\left(\mu + \alpha \cdot \sum_{t_n < t} e^{-\delta \cdot (t-t_n)}\right)$$

occurrence of one event triggers subsequent events



Generalised Hawkes likelihood?

In terms of a scorer, the Hawkes intensity is

$$\lambda \left(t; \{t_n\}_{n=1}^N \right) = F(s(t))$$
$$s(t) = \mu + \alpha \cdot \Phi(t)$$
$$\Phi(t) \doteq \sum_{t_n < t} e^{-\delta \cdot (t - t_n)}$$

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Can minimise a proper loss with this $s(\cdot)$ and Φ , and set

$$\lambda(t) = \frac{\Psi^{-1}(s(t))}{1 - \Psi^{-1}(s(t))}$$

Menon and Lee. Beyond the likelihood: new loss functions for (non-)linear Hawkes processes. In preparation.

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Can minimise a proper loss with this $s(\cdot)$ and Φ , and set

$$\lambda(t) = \frac{\Psi^{-1}(s(t))}{1 - \Psi^{-1}(s(t))} = F(s(t))$$

if we choose

$$\Psi^{-1}(v) = \frac{F(v)}{1 + F(v)}$$

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Hawkes process with linear $F(\cdot)$ For F(z) = z, we may explore losses with $\Psi(u) = \frac{u}{1-u}$

losses that directly seek density ratios
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losses that directly seek density ratios

One appealing candidate (Kanamori et al., 2009):

$$\ell(+1, v) = -v$$
 $\ell(-1, v) = \frac{1}{2}v^2$

• c.f. (Reynaud-Bouret 2014, Bacry et al., 2015)

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Potential closed-form solution

$$\boldsymbol{\theta}^* = \frac{N}{T} \cdot \left(\mathbb{E}\left[\Phi(\mathsf{T}') \Phi(\mathsf{T}')^T \right] \right)^{-1} \mathbb{E}\left[\Phi(\mathsf{T}) \right]$$

when this quantity is non-negative

Hawkes process with exponential $F(\cdot)$

For $F(z) = e^{z}$, we may explore losses with $\Psi(u) = \log \frac{u}{1-u}$

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One appealing candidate is familiar logistic loss

on nonlinear Hawkes with logistic regression!

Hawkes process with exponential $F(\cdot)$

For $F(z) = e^{z}$, we may explore losses with $\Psi(u) = \log \frac{u}{1-u}$

One appealing candidate is familiar logistic loss

on nonlinear Hawkes with logistic regression!

By weighting the negative class, this is actually equivalent to MLE

• follows from (Fithian & Hastie, 2013)

Illustration: fitting with proper losses

Prediction of # events on lastfm and bitcoin datasets



Summary thus far



Fairness-aware classification

Fairness-aware classification

Learn a classifier achieving two goals:

- accurately predict a target label
- don't discriminate on some sensitive feature



Fairness-aware classification: formally

We seek a classifier $f \colon \mathcal{X} \to \{\pm 1\}$, with induced predictions $\hat{\mathbb{Y}}$

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f should predict well target variable Y

• e.g. attain low balanced error,

$$BER(f) \doteq \frac{1}{2} \cdot \left(\mathbb{P}(\hat{Y} = +1 \mid Y = -1) + \mathbb{P}(\hat{Y} = -1 \mid Y = +1) \right)$$

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- f should predict poorly sensitive variable \overline{Y}
 - e.g. attain high balanced error,

$$\overline{\text{BER}}(f) \doteq \frac{1}{2} \cdot \left(\mathbb{P}(\hat{\mathbf{Y}} = +1 \mid \overline{\mathbf{Y}} = -1) + \mathbb{P}(\hat{\mathbf{Y}} = -1 \mid \overline{\mathbf{Y}} = +1) \right)$$

We seek a solution to

```
\min_{f} \operatorname{BER}(f) - \lambda \cdot \overline{\operatorname{BER}}(f)
```

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$$\begin{split} \min_{f} \mathrm{BER}(f) - \lambda \cdot \overline{\mathrm{BER}}(f) &= \min_{s} \mathop{\mathbb{E}}_{P} \left[\left[s(\mathsf{X}) < 0 \right] \right] + \mathop{\mathbb{E}}_{Q} \left[\left[s(\mathsf{X}') > 0 \right] \right] \\ &- \lambda \cdot \left(\mathop{\mathbb{E}}_{\overline{P}} \left[\left[s(\mathsf{X}) < 0 \right] \right] + \mathop{\mathbb{E}}_{\overline{Q}} \left[\left[s(\mathsf{X}') > 0 \right] \right] \right) \end{split}$$

We seek a solution to

$$\min_{f} \operatorname{BER}(f) - \lambda \cdot \overline{\operatorname{BER}}(f) = \min_{s} \operatorname{\mathbb{E}}_{P} \left[\left[s(\mathsf{X}) < 0 \right] + \operatorname{\mathbb{E}}_{Q} \left[\left[s(\mathsf{X}') > 0 \right] \right] - \lambda \cdot \left(\operatorname{\mathbb{E}}_{\overline{P}} \left[\left[s(\mathsf{X}) < 0 \right] + \operatorname{\mathbb{E}}_{\overline{Q}} \left[\left[s(\mathsf{X}') > 0 \right] \right] \right)$$

Natural to consider surrogate risk

$$\min_{s} \operatorname{BER}_{\ell}(s) - \lambda \cdot \overline{\operatorname{BER}}_{\ell}(s)$$

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Natural to consider surrogate risk

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but in general this will be non-convex

Alternately, let us consider the Bayes-optimal solutions

$$f^* \in \underset{f: \ \mathcal{X} \to \{\pm 1\}}{\operatorname{argmin}} \operatorname{BER}(f) - \lambda \cdot \overline{\operatorname{BER}}(f)$$

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$$\overline{\pi} \doteq \mathbb{P}(\overline{\mathbf{Y}} = +1) \qquad \pi \doteq \mathbb{P}(\mathbf{Y} = +1)$$

Just requires CPE on the target and sensitive features!

- tuning of λ does not require re-training
- also useful to study feature learning (McNamara et al., 2017)

Menon and Williamson. The cost of fairness in binary classification. https://arxiv.org/abs/1705.09055

Illustration of CPE approach

Competitive performance with bespoke optimisation (CDV) on UCI adult and synthetic Gaussian datasets



Conclusion

Talk summary

A formal link between DRE and CPE

CPE approach to three distinct learning problems



For another day



Collaborators









Brendan van Rooyen ANU

Bob Williamson ANU

Cheng Soon Ong Data61/ANU

Richard Nock Data61/ANU



Nagarajan Natarajan MSR Bangalore



Giorgio Patrini

UvA-Bosch DELTA







Lizhen Qu Data61/ANU

Thanks!

Further reading

Linking losses for density ratio and class-probability estimation. Aditya Krishna Menon and Cheng Soon Ong. ICML 2016.

A scaled Bregman theorem with applications. Richard Nock, Aditya Krishna Menon and Cheng Soon Ong. NIPS 2016.

Learning from corrupted binary labels via class-probability estimation. Aditya Krishna Menon, Brendan van Rooyen, Cheng Soon Ong and Robert C. Williamson. ICML 2015.

Learning with symmetric label noise: the importance of being unhinged. Brendan van Rooyen, Aditya Krishna Menon and Robert C. Williamson. NIPS 2015.

Learning from binary labels with instance-dependent corruption. Aditya Krishna Menon, Brendan van Rooyen and Nagarajan Natarajan. https://arxiv.org/abs/1605.00751

Making deep neural networks robust to label noise: a loss correction approach. Giorgio Patrini, Alessandro Rozza, Aditya Krishna Menon, Richard Nock, Lizhen Qu. CVPR 2017.

Beyond the likelihood: new loss functions for (non-)linear Hawkes processes. Aditya Krishna Menon and Young Lee. In preparation.

The cost of fairness in binary classification. Aditya Krishna Menon and Robert C. Williamson. https://arxiv.org/abs/1705.09055